Structural classification of the amide I sites of a beta-hairpin with isotope label 2DIR spectroscopy

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Supplementary Material for PCCP

Structural classification of the amide I sites of a β-hairpin with isotope label 2DIR spectroscopy

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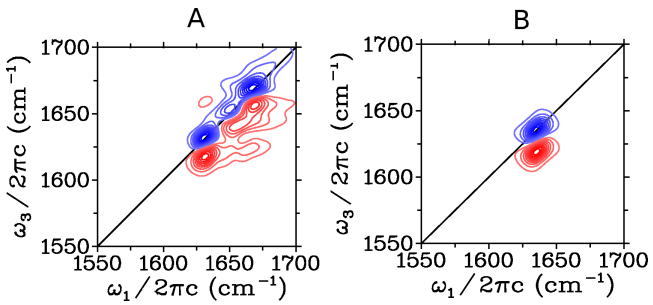

Fig. 1 S: 2DIR spectrum (parallel polarization) of trpzip2 with the T10 site labeled with $^{13}C^{16}O$ (A) and 2DIR spectrum of only the T10 site (B) at pH 2.5. A total of 18 equally spaced contours are plotted between $\pm$10% and $\pm$90% of the most intense peak. Blue contours are negative (simulated emission and bleaching) and red contours are positive (excited state absorption). In A, labeled spectrum for T10 is separated from the main spectrum of trpzip2 and is same as the spectrum for only the T10 site. Therefore, calculating the spectrum for only a particular site suffices for studying site-specific vibrational dynamics.

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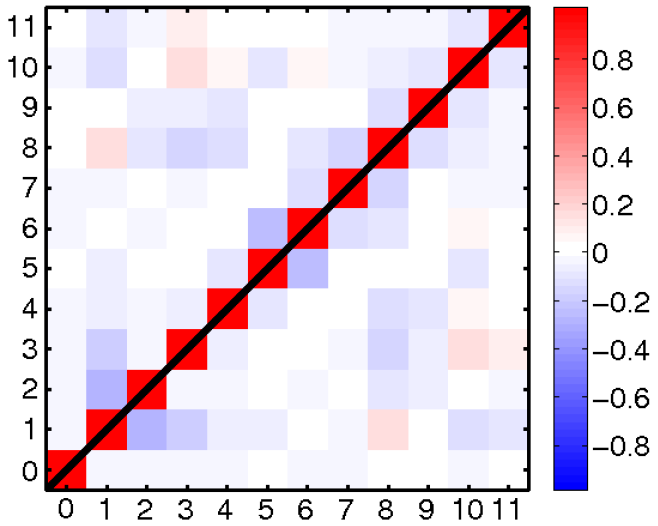

Fig. 2 S: Zero time cross-correlation plot for site frequencies. Red and blue correspond to correlation and anti- correlation, respectively.

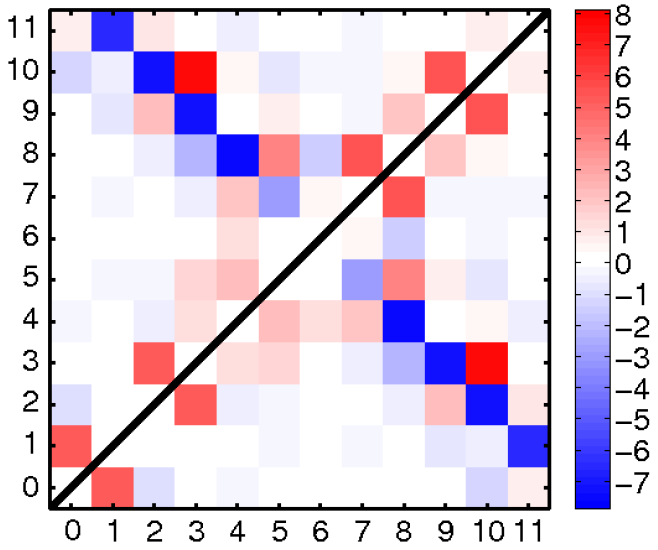

Fig. 3 S: Couplings (J_{ij}) among the sites: blue corresponds to a negative value, while red is positive. The most intense colors have the value of $\pm$ 7 cm^{-1}.

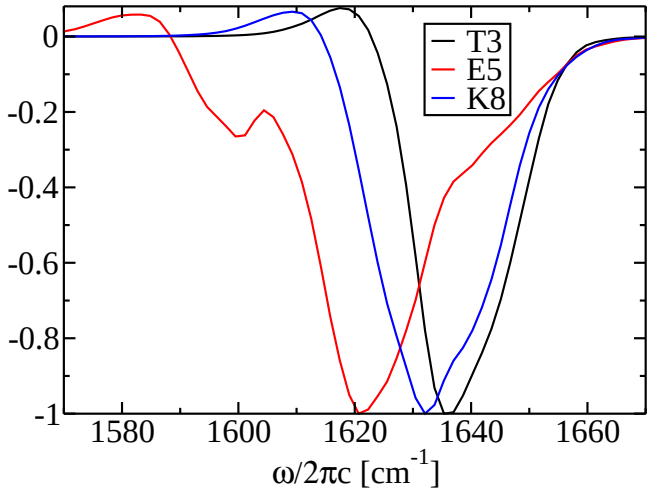

Fig. 4 S: Comparison of the diagonal slices of the 2DIR peaks of T3, E5, and K8.

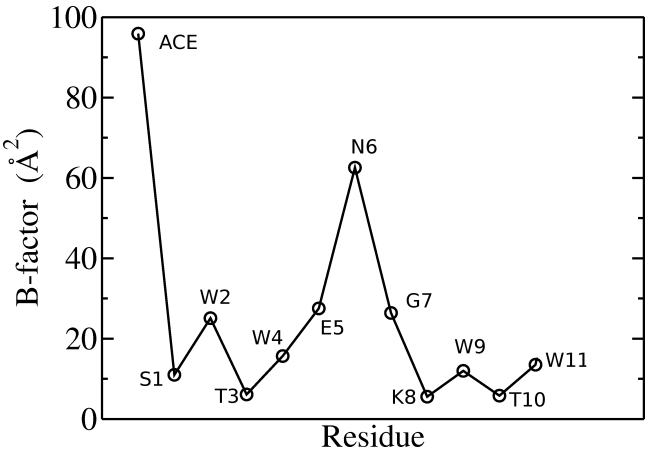

Fig. 5 S: B-factors of the peptide units of trpzip2.